

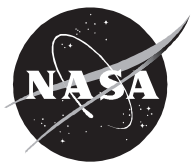
NASA/CR-2002-211460
ICASE Report No. 2002-7



Applicability of the Continuum-shell Theories to the Mechanics of Carbon Nanotubes

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April 2002

Report Documentation Page		
Report Date 00APR2002	Report Type N/A	Dates Covered (from... to) -
Title and Subtitle Applicability of the Continuum-shell Theories to the Mechanics of Carbon Nanotubes	Contract Number	
	Grant Number	
	Program Element Number	
Author(s) V.M. Harik, T.S. Gates and M.P. Nemeth	Project Number	
	Task Number	
	Work Unit Number	
Performing Organization Name(s) and Address(es) ICASE Mail Stop 132C NASA Langley Research Center Hampton, VA 23681-2199	Performing Organization Report Number	
Sponsoring/Monitoring Agency Name(s) and Address(es)	Sponsor/Monitor's Acronym(s)	
	Sponsor/Monitor's Report Number(s)	
Distribution/Availability Statement Approved for public release, distribution unlimited		
Supplementary Notes ICASE Report No. 2002-7		
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Subject Terms		
Report Classification unclassified	Classification of this page unclassified	

Classification of Abstract unclassified	Limitation of Abstract SAR
Number of Pages 21	

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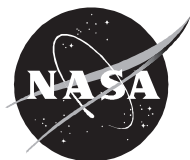
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Prepared for Langley Research Center
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APPLICABILITY OF THE CONTINUUM-SHELL THEORIES TO THE MECHANICS OF CARBON NANOTUBES

V. M. HARIK*, T. S. GATES† and M. P. NEMETH‡

Abstract. Validity of the assumptions relating the applicability of continuum shell theories to the global mechanical behavior of carbon nanotubes is examined. The present study focuses on providing a basis that can be used to qualitatively assess the appropriateness of continuum-shell models for nanotubes. To address the effect of nanotube structure on their deformation, all nanotube geometries are divided into four major classes that require distinct models. Criteria for the applicability of continuum models are presented. The key parameters that control the buckling strains and deformation modes of these classes of nanotubes are determined. In an analogy with continuum mechanics, mechanical laws of geometric similitude are presented. A parametric map is constructed for a variety of nanotube geometries as a guide for the applicability of different models. The continuum assumptions made in representing a nanotube as a homogeneous thin shell are analyzed to identify possible limitations of applying shell theories and using their bifurcation-buckling equations at the nano-scale.

Key words: carbon nanotubes, mechanical behavior, elasticity, buckling modes, scaling laws

Subject classification. Computational Materials Science

1. Introduction. Single-walled carbon nanotubes (NTs) are hollow cylindrical, shell-like macromolecules that are composed of carbon atoms arranged in periodic hexagonal cells [1]. Recent studies [1-6] indicate that these structures have great promise for providing superior mechanical properties such as stiffness approaching 1.5 TPa and strength approaching 100 GPa, with a density of about 1.3 g/cm³. However, because of their nanometer size, direct measurement of these NT properties has been found to be extremely difficult. A review of the recent literature shows that, to date, mechanical deformations of NTs have been examined via experimental characterization [1], while predicted properties have been determined by using *ab initio* (i.e., atomistic [2, 4]) methods or molecular dynamics (MD) simulations [3, 6]. To utilize both measured and calculated properties in the design of nanometer scale sensors and material systems with sub-micron inclusions, a full in-depth understanding of mechanical behavior of carbon NTs is required.

Representing new nanostructured materials with equivalent-continuum models also appears to be a viable approach to developing a means to describe their mechanical behavior. However, the applicability of any

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continuum model should be well defined. Toward that purpose, this study addresses the question: “Can continuum-mechanics models of NT behavior be used to determine their global response and, if so, what are the limitations?” This question arises naturally from the fact that NTs are cylindrical, lattice-like molecular structures and equivalent-continuum models [3, 7, 8-10] have been used recently to estimate global properties, such as shell stiffness [3, 7] and an equivalent thickness of the graphene lattice [10]. Meanwhile, it has also been demonstrated that representing a NT as a continuum shell implicitly imposes certain restrictions on the structural features of NTs. The assumption of a continuum cross-sectional area imposes certain structural and size limitations on nanostructures [5, 8], while the concept of shell stiffness may have to be re-defined as an intrinsic material constant without the use of NT thickness [7] when a classical shell model is used.

The global mechanical behavior of the carbon lattice can be also analyzed by representing the discrete molecular structure with an equivalent truss model and then as a homogeneous equivalent-continuum [10]. This representation is accomplished by exploiting the periodicity of the graphene sheet and establishing a correspondence between local quantities, such as the bond strength, with global properties, such as elastic energy. Such approach relies on equating the energies of the two corresponding systems. This method of achieving an equivalent continuum representation has been applied successfully to structural mechanics problems in the past for space applications, where vibration and buckling modes of reticulated, large-area lattice-structures have been modeled with classical and higher-order plate theories [11]. In some cases, local details were incorporated into high-order global structural theories through the use of micropolar-continuum models [12]. However, the meaningfulness of all of these continuum models depends on several basic assumptions about the relative wavelengths of the global structural deformations as compared to the characteristic dimensions of local structural features. In the context of NTs, the equivalence of the total energy of a molecular lattice with the elastic strain energy of an equivalent reticulated structure and with that of a continuum plate [10] or shell, and similarities in their kinematics appear to be the key issues.

To obtain meaningful values for the global mechanical properties of NTs, whose calculated values are based upon a structural theory, the applicability of the continuum model upon which the structural theory is based must be well defined at the nanometer scale and well understood. Toward that goal, one objective of the present study is to examine issues that typically arise in continuum modeling of discrete systems and continuum representation of NTs. Particular emphasis is placed on interpreting the limitations that are imposed on the continuum model by the underlying assumptions. Other objectives are to identify fundamental parameters that can be used to qualitatively identify limitations of continuum models and to provide a means for classifying nanotubes.

Continuum shell theories are of primary interest in the present study, and, thus, specific comments about the limitations of using shell buckling as a means for deducing mechanical properties are presented. Motivation for accomplishing these objectives stems, to a large extent, from mechanical problems associated with the deformation of NT-based sensors and scanning probes (e.g., atomic force microscope tips [13, 14]) that are used for material characterization. These mechanical problems and related issues include: 1) the ability of a given continuum model to describe adequately the deformation of molecular lattice-type structures, 2) how a NT is supported and how the load is introduced, 3) the effects of structural imperfections and deviations in cylindrical geometry, and 4) the accuracy of recorded measurements. For example, the introduction of mechanical loads into a NT-based probe may be affected significantly by the local graphene structure of the NT.

To accomplish the objectives of the present study, the structure and geometry of NTs are described first. Then, several issues about continuum modeling of NTs are presented and examined in detail. Next, four major classes of NTs that can be analyzed with equivalent-continuum models, under certain restrictions on the size of a NT and its strains, are identified. These classes include thin and thick NT shells, long NTs and NT beams. The key parameters that fully characterize the global behavior of NTs and scaling laws for NT buckling are derived *via* the scaling analysis of NT deformation and its structure. A parametric map for the four classes of nanotubes is constructed that can be used to link NT behavior to specific equivalent-continuum models, that can be used for data reduction in characterization [13, 14] and MD simulations [3]. Lastly, limitations of using a shell representation for NTs and classical shell theories to characterize NT global behavior are discussed and pitfalls are identified.

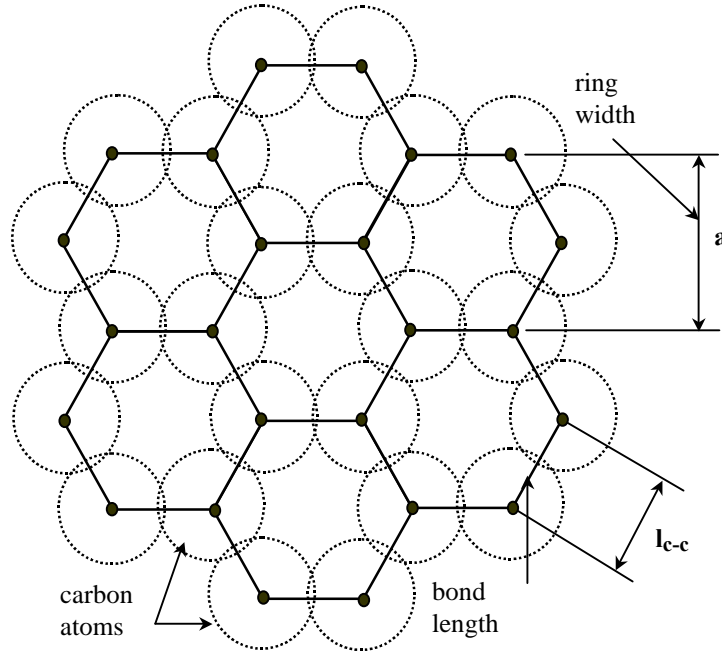


Figure 1. Schematic of a carbon lattice sheet composed of carbon atoms in a periodic hexagonal arrangement.

2. Continuum modeling issues at nanometer scale.

2.1. Nanotube structure. A carbon NT is composed of a cylindrical lattice-like sheet of carbon atoms. In the carbon sheet (Fig. 1), the adjacent carbon atoms are separated by the distance of about 0.14 nm, which is the length of the carbon-carbon/C-C bond, l_{c-c} . A NT consists of many hexagonal carbon rings that have a width, a , of about 0.246 nm [1]. These carbon rings are the structural cells in a NT. Different orientation of the carbon rings or cells determine their chirality and result in distinct NT structures (e.g., the “arm-chair” or “zig-zag” NTs). Current processing technologies produce nanotubes with wide variations in length, $1 \text{ nm} < L_{NT} < 10 \text{ }\mu\text{m}$, and radius, $0.2 \text{ nm} < R_{NT} < 10 \text{ nm}$. Since the ring width, a , is one of the smallest periodic elements in the NT lattice, it can be identified as the characteristic dimension associated with the local structure of a NT.

2.2. Continuum modeling of lattice-like structures. To address the shell-like deformation of NTs, the nanometer-scale structural features have to be properly accounted for in an equivalent-continuum model. In this section, some aspects of a shell-like representation of NTs are discussed to illustrate the origin and length-scale limitations of continuum mechanics assumptions. A careful description of familiar concepts is needed when they are applied at the nanometer-scale level.

In continuum mechanics, the material particles that comprise a deforming shell are contained within top and bottom bounding surfaces and edge faces. The middle surface of the shell is often used as the reference surface and all of the surfaces are assumed to be smooth. This simplified representation is motivated by the fact that a fully three-dimensional representation of the material body is not amenable to simplified solutions that are needed for practical engineering analysis and design studies. This two-dimensional, simplified representation of the material body is based upon the fact that two of its characteristic length dimensions are substantially larger than its through-the-thickness dimension. Moreover, the characteristic through-the-thickness dimension is presumed to be substantially larger than the characteristic dimension of the local structural details such as the C-C bond length, l_{C-C} . For carbon NTs, the thickness-to-bond-length ratio, h_{NT}/l_{C-C} , is not a large number, which points out the importance of molecular structure for NT behavior.

The NT shell-reference surface is a mathematical surface that connects all of the carbon atoms and provides a basic equivalent-continuum representation of a NT-shell without specifying the value of NT thickness, h_{NT} . It is difficult to define accurately the thickness of a NT due to the discrete nature of NT structure and, thus, the effective NT thickness, h_{NT} , can only be estimated by using various assumptions [3, 7, 8, 10]. This point is important because NT thickness is a key geometric parameter that is needed to characterize the range of NT structures that can be analyzed with different continuum shell theories. Even in the simplest continuum models, the global bending stiffness of a shell is proportional to the cube of the shell thickness. In addition, the thickness-to-radius ratio is known to be important in the formulation of shell theories [15, 16].

Nanometer-scale effects may introduce corrections to NT geometry such as: 1) variations in the estimates of the effective thickness of NTs, which influence the value of the thickness-to-radius ratio h_{NT}/R_{NT} , 2) the NT radius, R_{NT} , is uniquely defined only when the aforementioned reference shell-surface is used, and 3) the value of NT length, L_{NT} , is subject to the end-cap effects that have the length-scale on the order of NT radius or $a/2$ for the NTs with open ends (Fig 2). These ambiguities in NT geometric parameters and the NT open-lattice structure characterize the “effective” geometries of NTs that are marked by dotted lines in Fig. 2. The issue of effective NT thickness is related to the issues regarding the use of other concepts such as a volume and a volume fraction at the nanometer scale. A difference in the definitions of these concepts may lead to some variations in the numerical results.

2.3 Applicability criteria for continuum models. At the nanometer scale, the applicability of continuum models to NT behavior can be qualitatively evaluated by examining the validity of continuum-based assumptions and identifying model restrictions related to geometric parameters of NT structure and its deformation. Before a continuum model is used, three basic criteria have to be satisfied. First, a homogenization criterion, such as $L_{NT}/a > 10$, for property averaging should be established. This criterion provides a measure of relevance of the local lattice to the global NT structure. Second, linearity of elastic strains should be enforced, i.e., the axial strain, ϵ_s , must be

small compared to unity. For NT shells, this range of small strains is limited from above by 2-5% [3, 6]. The strain value under bending or compressive loading can be bounded by the maximum-strain criterion:

$$\varepsilon_x \approx (L_{NT0} - L_{NT})/L_{NT0} \ll 1, \quad (1)$$

where L_{NT0} and L_{NT} are the original or non-deformed length of a NT and the deformed length, respectively. Moreover, all strains should be smaller than the lowest estimate of the NT thickness. The third basic criterion is that geometrically linear models are restricted to small deflections of long NT structures.

3. Classification of nanotubes and key parameters. Separation of NTs into different classes is, to a large extent, a necessary step in developing appropriate models for various molecular structures. This classification is usually done by first identifying the key parameters that relate the local structural features to the global response. These geometric parameters may be used to capture the influence of NT structure on the degree of applicability of continuum shell models and the associated ranges of validity. After the key geometric parameters of NT structure are established, dimensional analysis is used to identify a few non-dimensional parameter-groups that fully characterize the dominant mechanical properties of the different classes of NTs.

Following classical shell theory [15, 16], the NT thickness-to-radius ratio restriction $h_{NT}/R_{NT} < 1/20$ can be used to loosely determine if a NT shell is thin and thus whether transverse shear can be neglected in the continuum shell model. Consideration of the length-to-radius restriction $L_{NT}/R_{NT} \gg 1$ will further define high aspect ratio NTs that have unique deformation modes. These restrictions can be used to group NTs into four classes; that is thin NT shells (class Ia), thick NT shells (class Ib), long NTs or high aspect ratio NTs (class II), and thin beam-like NTs or NT beams (class III) such that the normalized radius is $R_{NT}/a \approx 1$, where a is the side length of a carbon ring or cell (Fig. 2). This classification of NTs separates NT structures into groups that have similar global structural behavior, overall material properties and deformation modes.

The NT shell classes include the thick shells (class Ib) defined by the ratio $h_{NT}/R_{NT} > 1/20$, as the NT radius decreases to $R_{NT}/a \approx 2$. As soon as NT length, L_{NT} , becomes large so that the length-to-radius ratio L_{NT}/R_{NT} is well above 10, NTs acquire a high aspect ratio (class II) and the associated structural properties (e.g., low bending stiffness), but still behave like shells. Here, the value 10 is used to show at least an order of magnitude difference in the separation of the transverse and longitudinal dimensions or scales in NT structures. Such separation is based on inequalities and, thus, is not precise, of course. Note that the NT beams (class III) often also have high aspect ratios. The unique feature of NT beams is that the high curvature and the van der Waals forces inside of a NT become significant as far as structural properties and deformation are concerned [4, 8, 9]. As a result, the effective NT thickness is higher for NT beams. This increase in the effective NT thickness increases the value of the ratio, h_{NT}/R_{NT} , for shells or the ratio, h_{NT}/l_{C-C} , for the carbon lattice. The thin-shell models, which are based on classical shell theories [15, 16], are applicable only to two of the NT classes (i.e., class Ia and class II) with certain restrictions on NT size and the magnitude of its strains.

The name of each NT class is a reflection of the structural properties of NTs. That is, NT shells (class Ia and Ib) behave like either thin shells or thick shells (i.e., hollow cylinders). The long NTs of class II have a structural response that is similar to hollow columns regardless of the values of the NT radius. The NT beams deform like

either long beams or short beams (i.e., solid cylinders). The name of each NT class also indicates which models may be applicable to characterize the NT global behavior. Variations in the loading conditions may introduce only minor refinements into applicability of these models.

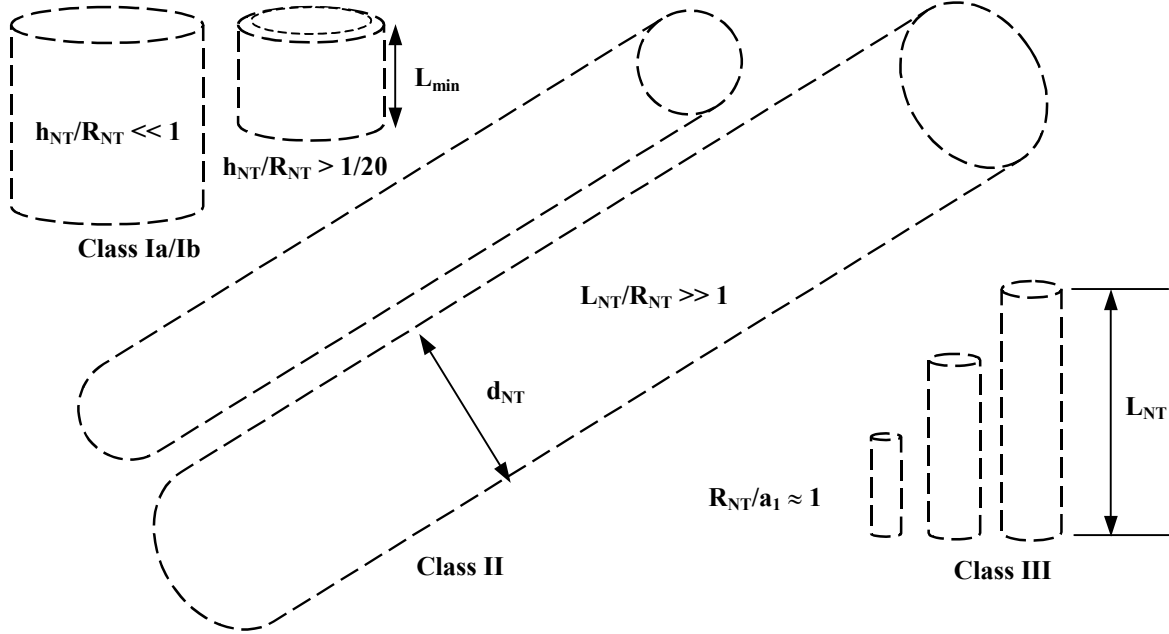


Figure 2. Schematics of the “effective” NT geometries (dotted lines) for the four classes of NTs: thin and thick NT shells, long NTs or high aspect ratio NTs, and NT beams.

4. Effects of nanotube structure on deformation. The categorizing of NTs into different classes indicates that NT structure may have significant influence on their mechanical response (i.e., their deformation modes for the shell-like and beam-like geometries). The mechanical problems associated with the deformation of NT-based sensors and scanning probes [11, 12] also require selection of appropriate models for various NT geometries. For NT probes, a typical device involves a NT attached to a sharp tip of a cantilever beam, which is brought into close proximity or contact with the material tested and subjected to compression or bending. Here, deformation of NT shells is examined to illustrate the effect of NT structural parameters on their global response under compressive loadings.

Beam-like buckling modes of NTs subjected to axial compression depend on their geometry. Variations in the geometric characteristics of NT structure may also require examination of the shell-like buckling modes. This section shows how the applicability criteria for continuum models and the NT classes affect the analysis of NT buckling. This analysis is carried out for the three NT classes: Ia, Ib and II. Dimensional analysis of the shell buckling process was conducted, like that in Refs. [8, 9]. The analysis clearly identified the key geometric parameters that significantly affect the NT buckling behavior, i.e., the thickness-to-radius ratio, h_{NT}/R_{NT} , and the

aspect ratio, L_{NT}/R_{NT} . The following sections examine the effects of NT thickness, h_{NT} , and NT length, L_{NT} , on NT buckling predictions.

4.1. Effects of thickness estimates on nanotube buckling. For NT shells in class I, a linear analysis of shell buckling can be carried out with a modification of the classical formula [3, 13] for continuum shells. However, the range of NT structural parameters should be properly limited before such a model is used. First, according to the proposed homogenization criteria ($L_{NT}/a > 10$), the range of values for NT length should be limited from below by the minimum length, L_{min} . This criterion ensures unique averaging of NT material properties. Second, the range of values for NT radius depends on the choice of thin or thick NT shells. That is, the buckling strain of the thin NT shells can be approximated by the following modified formula

$$\epsilon_{cr} = \frac{1}{\sqrt{3(1-\nu^2)}} \left(\frac{h_{NT}}{R_{NT}} \right), \quad (2)$$

only when the inequality $h_{NT}/R_{NT} < 1/20$ is satisfied and NTs have moderate aspect ratios. Here, ν is Poisson's ratio. The original buckling formula [15] is not based on the non-dimensional quantity, h_{NT}/R_{NT} . It also includes the moment of inertia, I_{NT} . The later parameter was shown to be a dependent quantity in the dimensional analysis [8, 9]. At the nanometer scale, the mechanical strains are easier to define than the stresses, as indicated by the Eq. (2). In contrast to stresses, the global NT strains can be measured directly. The approximate nature of this equation is not only because of the assumption of linearity, but also because of the known sensitivity of shell buckling to small variations in thickness, cylindrical geometry and other nonlinear geometric effects [15, 16]. A formula similar to Eq. (2) without a non-dimensional ratio has been used in MD simulations but without any restrictions or analysis [3].

The buckling predictions of Eq. (2) strongly depend on the NT thickness estimates, which have been bounded between the MD prediction of 0.066 nm, which is based on a shell analogy [3], and the value of graphite interlayer spacing, t , of about 0.34 nm. The magnitude of interlayer spacing is affected by the van der Waals forces and applied pressure [1]. An intermediate estimate of 0.072 nm is based on a bond-thickness estimate [8], while an equivalent-truss model [10] for the planar carbon lattice-sheets yields an estimate of 0.28 nm. The effect of such variations in thickness estimates on the buckling behavior of NT shells is illustrated in Fig. 3. Note that the criterion for the maximum strains (2-5%) imposes an upper bound or a cut-off boundary for the curves in Fig. 3 that represent different estimates of NT thickness and span a range of values of the NT radius.

Equation (2) provides a *structure-property relationship* that connects the critical buckling strain to the structural characteristics of NTs (i.e., h_{NT} and R_{NT}), for the aspect ratio, L_{NT}/R_{NT} , that is not large. Note that Eq. (2) involves only one non-dimensional geometric quantity, h_{NT}/R_{NT} , which is identified as a key parameter that controls the NT buckling behavior. Poisson's ratio is a material constant for the class of NT shells. Therefore, NTs having the same value of the non-dimensional ratio h_{NT}/R_{NT} must have identical critical strain and buckling modes even if the individual parameters (i.e., h_{NT} and R_{NT}) are different. The last statement constitutes a *mechanical law of geometric similitude* for the class Ia of NT shells that have no imperfections. It is analogous to the laws of similitude in

continuum mechanics. Note that in classical mechanics, similitude is usually based on the analysis of differential equations as opposed to a parameter-group analysis.

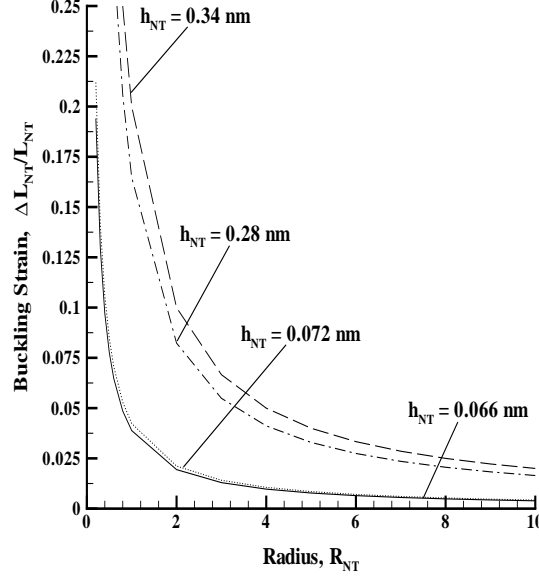


Figure 3. Dependence of the critical buckling strain of carbon NTs on their radius, R_{NT} (nm), for various estimates of the effective NT thickness, h_{NT} .

4.2. High aspect-ratio effects on nanotube buckling. The length of nanotubes affects their buckling strain and the associated deformation modes. For the class II of NTs with high aspect ratio, L_{NT}/R_{NT} , the critical axial strain, ϵ_{cr} , is proportional to the NT end-displacement and depends on the NT half-perimeter, πR_{NT} , normalized by the NT length, L_{NT} :

$$\epsilon_{cr} = \frac{1}{2} \left(\frac{\pi R_{NT}}{L_{NT}} \right)^2 \approx \frac{\Delta L_{cr}}{L_{NT0}} \quad (3)$$

if $L_{NT}/R_{NT} > 10$, or better yet, if $L_{NT}/d_{NT} > 10$, where d_{NT} is the diameter of a NT. Here, ΔL_{cr} is the critical end-displacement, $\Delta L = L_{NT0} - L_{NT}$. The difference in the two last inequalities points out that there exists a range of transitional values where Eq. (3) has marginal applicability. In some cases, a weighting factor may be also used to address specific structural properties. The factor “1/2” in Eq. (3) depends on the end conditions [15]. Here, the NT ends are simply supported. For the fixed ends, the critical strain is 4 times larger. Also, the moment of inertia, $I = \pi R^3 h$, the area, $A = 2\pi R h$, Young’s modulus and the mechanical stress are not explicitly used in Eq. (3), in contrast to the equation in Ref. [15]. Molecular dynamics (MD) simulations have confirmed a similar relation for a particular case of NT geometry [3].

Under compression, long NTs (class II) have the global deformation mode similar to that of nanometer-scale beams (class III, [8, 9]), because of their column-like structural properties associated with the high aspect ratios. However, the wall thickness effects reduce the critical strain by a half (see factor “1/2” in Eq. (3)). An initial bending would further decrease the value of the critical strain. The long NT shells are not as sensitive to

imperfections in the wall thickness as the NT shells in class Ia. However, the aforementioned ambiguities in the values of NT lengths and radii at the nanometer scale may also introduce some variations into the buckling predictions.

Eq. (3) also provides a *structure-property relationship* that connects the critical buckling strain or the critical end-displacement to the structure of long NTs, for which the aspect ratio is such that $L_{NT}/d_{NT} > 10$. Note that Eq. (3) also involves one non-dimensional quantity, R_{NT}/L_{NT} , which is a key non-dimensional parameter that affects the buckling behavior of NT shells. As a result, NTs having the same values of nondimensional ratio R_{NT}/L_{NT} must have identical critical strain and buckling modes, even if the individual parameters R_{NT} and L_{NT} are different. As mentioned before, this statement is also a *mechanical law of geometric similitude* for long NTs of the class II [8, 9], and is an extension of the laws of similitude from continuum mechanics. The buckling deformation of NTs described by Eq. (3) is identical to the buckling behavior of long NT beams.

4.3. Bending of nanotube shells. Bending is one of the dominant deformation modes of NT-based scanning probes. The effective bending modulus, E_{eff} , of a thick NT shell can be estimated by a formula [15]:

$$\frac{E_{eff}}{E_C} \propto \left[\left(1 + \frac{1}{2} \frac{h_{NT}}{R_{NT}} \right)^4 - \left(1 - \frac{1}{2} \frac{h_{NT}}{R_{NT}} \right)^4 \right] \quad (4)$$

where E_C is the effective Young's modulus of the carbon lattice [10]. Bending of thin shell-like structures is sensitive to the local curvature and other geometric parameters. For a thin cylindrical shell under bending loads, one side is compressed before buckling occurs at the local critical curvature, κ_{cr} . Then the local strain, $\epsilon_{cr} = \kappa_{cr} R_{NT}$, can be estimated by the Eq. (2) if the inequality $h_{NT}/R_{NT} < 1/20$ is satisfied. As a result, the critical curvature, κ_{cr} , is such that $\kappa_{cr} \propto (R_{NT})^{-2}$. This estimate is the same as that obtained by the MD simulation [3]. However, the key non-dimensional parameter, h_{NT}/R_{NT} , is confirmed by the dimensional analysis, so the relation $\kappa_{cr} \propto (h_{NT}/R_{NT})^2$ is more appropriate.

The approximate nature of continuum-based models is more evident in the analysis of buckling of NT shells caused by ambient pressure. The lateral pressure on a NT exerted by the surrounding molecules of a polymer or other matrix is likely to be non-uniform and discrete in nature. A shell-based model yields an estimate for the critical lateral pressure [15]: $P_{cr} \propto (h_{NT}/R_{NT})^3$. Note that the bending stiffness of shells is proportional to $(h_{NT})^3$. Applicability of this approximation is restricted by both the thin-shell assumption, $h_{NT}/R_{NT} < 1/20$, and the concept of “pressure” that requires large lateral area (or large R_{NT}). However, the robustness of this estimate is underscored by the fact that the same dependence is predicted for buckling caused by a discrete lateral force [15]. Notice that the expressions presented here depend only on the key nondimensional parameter, h_{NT}/R_{NT} , which is indicative of a shell approximation.

5. Limitations of continuum shell models. Equivalent-continuum models may be very useful for determining the global response and effective properties of nanotubes, at least for a limited range of geometric parameters.

However, it is essential to examine their ranges of validity and how the macroscopic assumptions are applied at the nanometer scale.

5.1. Limitations of continuum shell representation. In applying continuum shell theories to NTs, many of the same considerations that were examined for reticulated lattice structures must be addressed [11, 12]. Similar to other open lattice structures, NTs are characterized by the effective thickness. Even for the most basic continuum shell theory, the bending stiffness is proportional to the cube of the wall thickness. Thus, adequate representation of NT wall thickness is essential to the success of an equivalent-continuum model.

Another issue that must be considered for NTs is the contribution of the geometry of the periodic hexagonal cell to the definition of the equivalent-continuum stiffnesses. For example, studies on the homogenization of plate-like lattices made of beam-based cells indicate that equivalent stiffnesses are highly dependent on the cell geometry [10-12]. In addition, the cell geometry is typically manifested in the equivalent-continuum model as membrane and flexural orthotropies. As the n -fold symmetry (geometry and material composition) of a cell increases, the corresponding stiffnesses approach those for an isotropic material.

Load introduction is another important consideration in continuum modeling of NTs. Specifically, improper load introduction may precipitate local deformation that propagate through the NT, rendering equivalent-continuum models meaningless.

5.2. Limitations of classical shell theory. To examine possible length-scale limitations of macroscopic shell theories, all underlying continuum-based assumptions must be scrutinized. For convenience, these assumptions as applied to NTs are listed here:

- S1) the equivalent shell for a NT molecule deforms elastically,
- S2) the length, L_{NT} , and the width or the half-perimeter, πR_{NT} , are much larger than the shell thickness, h_{NT} , so that a two-dimensional theory sufficiently captures the dominant response,
- S3) the direction of the applied load remains constant during deformation (this essentially guaranties a conservative buckling problem),
- S4) the radius, R_{NT} , and the cross-section of the NT shell does not vary along the length,
- S5) elastic strains and rotations of the shell are small compared to unity, or the gradients of displacements are infinitesimal,
- S6) material line elements that are straight and perpendicular to the shell reference surface remain that way during deformation and are inextensible (i.e., Kirchhoff's hypothesis).
- S7) displacements are small compared to the shell thickness, h_{NT} ,
- S8) through-the-thickness normal stresses are negligible compared to other elastic stresses.

In classical continuum shell theory, all these assumptions are to be satisfied. In the context of NT mechanics, the range of validity of these different assumptions may be defined by using the geometric parameters of the NT molecular structure. This approach provides a link between the structure of carbon NTs, their mechanical behavior, and the shell model for the NTs.

In this study, the analysis is restricted to elastic behavior of the NT shells (assumption (S1)). Note that the bifurcation-buckling equations are linear [15]. The shell buckling theory that they come from is nonlinear [16], because the process of buckling is a nonlinear phenomenon. Assumption (S2) allows the use of two-dimensional theory for capturing the dominant global response features and in deriving the elastic shell equations. It is satisfied if the NT radius is such that $h_{NT}/R_{NT} < 1/20$. Assumption (S3) restricts the direction of displacement of carbon atoms located near the NT edges. Requirement (S4) about the constant radius and cross-sectional area leads to the constant moment of inertia. This requirement is a significant simplification since the NT structure is similar to the open lattice-type structures having many periodic cells. Note that assumptions (S3) and (S4) are not just shell assumptions, as they are used in the classical beam theory as well [8, 9].

Assumption (S5) implies that the shell cross-sections do not deform in their planes, instead, they remain perpendicular to the original image of the shell reference surface during axial deformation as required by assumption (S6). Kirchhoff's hypothesis (S6) can be linked to the elastic constitutive relation. To restrict stresses according to assumption (S8) is problematic for NTs of small radii. These stresses are noticeable for the NT diameters in the range $d_{NT} < 1$ nm [4], however, their magnitude diminishes as the diameters of NTs increase. These curvature-generated internal stresses set a lower limit on NT radius as far as the applicability of the thin-shell model is concerned.

5.3. Limitations of Donnell's equations. Selection of a set of shell buckling equations must be made with care, after an acceptable loading procedure has been developed. Donnell's shell equations have been used for NT buckling [7], however, it should be pointed out that these equations are more applicable to calculating linear-bifurcation points for cylinders that have more than two circumferential waves in the buckling pattern. Thus, Donnell's equations [16] do not predict the column-like buckling mode and would lead to errors if used for the analysis of long NTs. For instance, the limiting equation, Eq. (3), for critical strains cannot be achieved. To get the global column-buckling mode for long cylinders, a set of equations such as Flugge's equations must be used [16].

For both sets of bifurcation-buckling equations, it is important to note that the bifurcation (buckling) modes that are predicted are not the deformation mode exhibited by the buckled shell after the transient dynamic response of buckling has attenuated. The mode that is observed is the stable postbuckling mode. The bifurcation mode is unstable and is one of the configurations that the shell passes through on its way to the stable postbuckling configuration. This behavior is signified by the unstable nature of the bifurcation point. Thus, one must be cautious about drawing conclusions about the behavior of nanotubes from bifurcation buckling modes.

5.4. Nanotube buckling and characterization. The shell-like buckling of a NT has been used as a means for determining properties such as the axial stiffness or the effective elastic modulus of a nanotube [3]. Several considerations must be taken into account when using this technique in order to avoid significant errors in the calculated results. First, buckling loads of circular cylindrical shells are known to be highly sensitive to imperfections, such as initial geometric imperfections in the form of wall undulations, for some loading conditions. A detailed account of the effects of various imperfections on the buckling of compression loaded cylindrical shells is found in Ref. [18].

For uniform-compression-loaded cylinders, this sensitivity is manifested by unstable, symmetric bifurcation behavior with a multiplicity of eigenvalues that have the same numerical value. The multiplicity of eigenvalues corresponds to the presence of several unstable equilibrium branches that intersect the equilibrium path of the unbuckled shell. Moreover, the multiplicity of eigenvalues is an artifact of the high degree of axial symmetry exhibited by additional factors such as: 1) the geometry of the perfect shell, 2) the material composition, and 3) the loading and support conditions. The common intersection of the multiple unstable postbuckling equilibrium paths is manifested physically for a geometrically imperfect shell by the presence of a limit point of the equilibrium path with a magnitude that is usually much smaller than the magnitude of the corresponding bifurcation point. Differences between buckling loads obtained from bifurcation analyses for geometrically perfect shells and from nonlinear analyses of imperfect shells, which agree well with experiments, are known to be as large as 60%. Thus, mechanical properties that are based on calculated bifurcation buckling loads may be substantially in error.

Second, for other loading conditions such as torsion, the imperfection sensitivity of a circular cylinder may be much less severe than that exhibited by the corresponding compression-loaded shell. This reduced sensitivity results from the fact that for torsion loading, the shell experiences zones of diagonal tension incipient to buckling and is not dominated by compressive stresses. For a loading such as pure bending, a reduction in imperfection sensitivity occurs because of the absence of axial symmetry and the fact that the shell is again not dominated by compressive stresses. This lack of symmetry is typically manifested mathematically by distinct bifurcation points or eigenvalues (no multiple path intersections). However, modal interactions that lead to imperfection sensitivity may occur for cases in which the distinct eigenvalues are nearly equal. Altogether, these observations suggest that nanotube loading conditions that are not compression dominated may yield better measures of mechanical properties.

5.5. A role of the structural-response scale. Guidelines for the range of validity of a given continuum model must be also established with respect to the characteristics of the global mechanical response. To define the range of validity of shell theories, for isotropic-material bodies, the parameter h/l is used [17], where h is the nominal or maximum shell thickness and l is the characteristic dimension of the expected shell response. For example, l could be the wavelength of a buckling or vibration mode. It may also be taken as the minimum radius of curvature of the two-dimensional shell surface, which implies a relatively large wavelength response. As a result, the role of the ratio h/l is similar, but not identical, to that of the thickness-to-radius ratio. Consequently, a rough guideline for defining the applicability of classical thin-shell theory to structural-response problems is that h/l must be less than or equal to $1/20$. Naturally, this is similar to the requirement on the thickness-to-radius ratio. As one might expect, for high-frequency buckling or vibration modes, classical thin-shell theory may be inadequate.

As one might also expect, the need to analyze relatively thick isotropic and thin anisotropic shells arises in engineering applications. For many of these cases, the guideline $h/l \leq 1/20$ generally doesn't apply and a more robust measure is needed to gage the applicability of thin-shell theory. Even for thin anisotropic shells, a measure such as $(h/l)M \leq 1/20$ is needed, where M is a material-system weighting factor that accounts for how the relative stiffnesses of the material system affect the range of validity of thin-shell theory. For all cases, when a measure like $(h/l)M$ gets relatively large, a refined shell theory is very likely needed to get accurate predictions of the structural response. This requirement for a refined theory can become even more important when the response desired is a

localized quantity like a stress or strain, as compared to a global quantity like a buckling load or a fundamental vibration frequency.

5.6. Other important shell parameters. Classical thin-shell theory suggests that there is another important parameter, which is useful for classifying the global mechanical behavior of NTs, besides the length-to-radius ratio L_{NT}/R_{NT} and the thickness-to-radius ratio, h_{NT}/R_{NT} . That is, the Batdorf Z parameter: $Z \sim L^2/(Rh)$, or $Z \sim (L/R)^2(R/h)$ [19]. This parameter is proportional to the product of the aforementioned key non-dimensional parameters. The derivation of the Batdorf Z parameter is based on a dimensional analysis of Donnell's simplified equations [16] for buckling of thin-walled circular cylindrical shells. This parameter can be also used to characterize the influence of geometry on global buckling behavior of compression-loaded circular cylindrical shells.

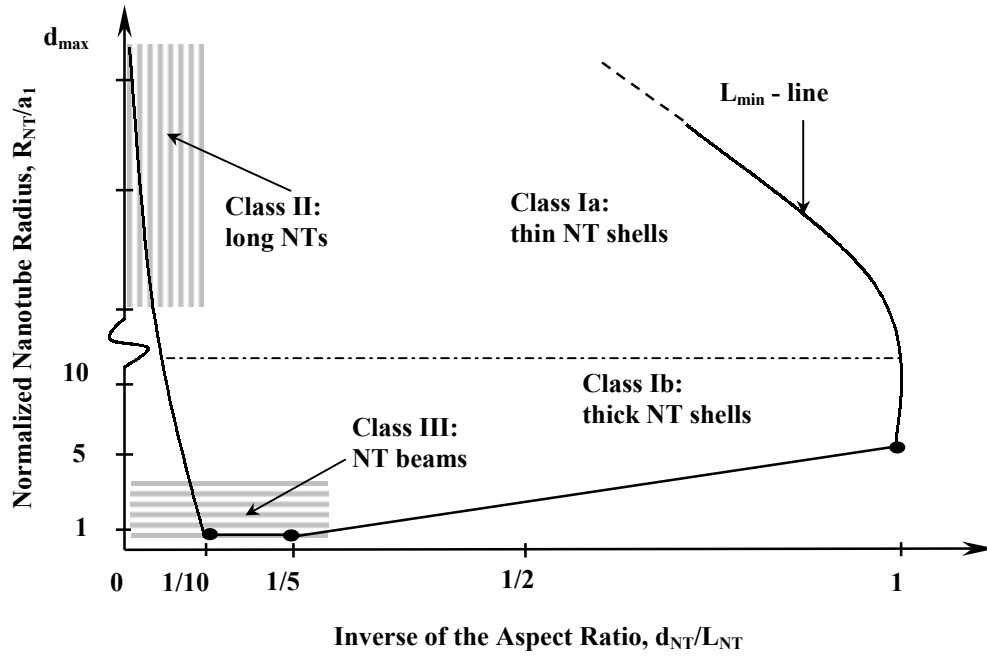


Figure 4. A model applicability map (MAM) with the ranges of values for non-dimensional geometric parameters that define NT classes and indicate the limits in the applicability of the thin-shell model for NTs.

5.7. A model applicability map. The aforementioned analysis can be used to construct an applicability map for thin-shell models for the classes Ia and II of carbon NTs (Fig. 3). These classes of NTs are defined by dimensional restrictions on NT geometric parameters, which are formulated with inequalities that allow one to consider wide ranges of numerical values for the NT parameters. Ranges of values for the inverse of aspect ratio, L_{NT}/d_{NT} , and the normalized radius, R_{NT}/a , are marked for each class of NTs. The L_{min} -line is based on the homogenization criteria $L_{NT}/a > 10$. The model applicability map shown in Fig. 4 provides guidance for MD simulations and experiments, for possible size effects in the thin-shell model that may be used for data reduction.

The descriptive name of each NT class indicates the structural properties of NTs as well as the potential continuum models that can be used to predict their global mechanical behavior. That is, NT shells behave like either thin shells or thick shells depending on the thickness-to-radius ratio, h_{NT}/R_{NT} . The long NTs (class II) have structural

behavior that is similar to the behavior of columns. The NT beams deform like macroscopic beams. As a result, the map in Fig. 4 can be used to help find out what basic models are appropriate to describe the overall mechanical behavior of NTs in a particular class. The applicability map (Fig. 4) also indicates that simple shell models may be ineffective for the parameters along the limiting lines on this map. For example, micropolar effects [12] may be significant along the L_{min} -line where higher-order theories may be required.

6. Summary and discussion. The *structure-property relationships* that relate the critical strains to NT structure have been examined and four broad classes of carbon NTs have been identified. These classes include thin and thick *NT shells*, *high aspect ratio NTs*, and *NT beams*. The importance of classifying the types of NT structures has become apparent when the shell-like buckling of NTs was investigated. In each class, NTs have unique buckling behavior. The scaling analysis is used to identify the key parameters that control the buckling behavior of each class of NTs. It has been shown that NTs having the same values of non-dimensional ratios (h_{NT}/R_{NT} for NT shells and L_{NT}/R_{NT} for long NTs) must have identical critical strain and buckling modes even if the individual parameters are different. This constitutes the scaling laws of geometric similitude.

Nano-scale effects and other key conclusions are summarized here as follows:

- 1) there are variations in the estimates of the effective thickness of carbon nanotubes;
- 2) the nanotube radius is uniquely defined only when the reference shell-surface is used;
- 3) the value of nanotube length is subject to the end-cap-effects;
- 4) the axial strain of a nanotube is easier to define than its stresses;
- 5) displacements on the ends of NTs are easier to implement than tractions as boundary conditions;
- 6) the hyperelastic behavior of a nanotube extends the typical 2% limit for the elastic strain of solids;
- 7) carbon nanotubes of small radii behave as beams;
- 8) a homogenization criterion ($L_{NT}/a_l > 10$) is required;
- 9) the moment of inertia is a dependent parameter in the buckling formulae for nanotubes;

A model applicability map for the four classes of NTs is constructed to link NT behavior to specific equivalent-continuum models that can be used for data reduction and NT probe designs. The approximate nature of the analysis may provide potential sources of errors in the characterization of NT behavior and mechanical properties. For instance, the bending stiffness of shells is highly sensitive to the thickness, h_{NT} , and its variations. Its value is proportional to $(h_{NT})^3$. As a result, the compression-loaded cylindrical structures are very sensitive to small deviations in their wall-thickness (they can be less than one wall-thickness) and global properties that are calculated by using buckling loads could be in error of as much as 60%.

7. Concluding remarks. Issues that should be addressed when using an equivalent-continuum model to represent the global mechanical behavior of a carbon nanotube have been examined in the present study, in detail. In addition, applicability criteria have been discussed, fundamental parameters have been identified, and a means for classifying nanotubes has been presented. Moreover, four broad classes of carbon nanotubes have been identified that include thin and thick shell-like structures of moderate aspect ratio, high-aspect-ratio shell-like structures, and

beam-like structures. Additionally, a parametric map that links the four classes of nanotubes with the specific types of continuum models has been presented.

The buckling behavior of carbon nanotubes has also been a primary focus of the present study. Structure-property relationships that relate the critical strains to the nanotube structure have been established that apply to the three broad classes of carbon nanotubes defined herein. For each nanotube class, a unique buckling behavior has been identified and a scaling analysis was used to identify the fundamental non-dimensional parameters that control the buckling behavior for each nanotube class. Moreover, the corresponding scaling laws of geometric similitude have been described. For nanotubes with the same values of the non-dimensional parameters, it has been shown that they must have identical critical strain and buckling modes, even if the individual structural features are different. As a result, the analysis presented herein may help to reduce the number of molecular dynamics simulations that are needed to describe a whole class of NTs.

Acknowledgements. Research of V. M. Harik is funded by the NASA Langley Research Center under Contract NAS1-97046. Discussions with Drs. D. Ambur and J. Reeder (NASA LaRC) and members of the NASA Nanotechnology Team are greatly appreciated.

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE April 2002		3. REPORT TYPE AND DATES COVERED Contractor Report
4. TITLE AND SUBTITLE Applicability of the continuum-shell theories to the mechanics of carbon nanotubes			5. FUNDING NUMBERS C NAS1-97046 WU 505-90-52-01	
6. AUTHOR(S) V.M. Harik, T.S. Gates, M.P. Nemeth				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) ICASE Mail Stop 132C NASA Langley Research Center Hampton, VA 23681-2199			8. PERFORMING ORGANIZATION REPORT NUMBER ICASE Report No. 2002-7	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Langley Research Center Hampton, VA 23681-2199			10. SPONSORING/MONITORING AGENCY REPORT NUMBER NASA/CR-2002-211460 ICASE Report No. 2002-7	
11. SUPPLEMENTARY NOTES Langley Technical Monitor: Dennis M. Bushnell Final Report To appear in the Proceedings of the AIAA SDM Conference.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Unclassified-Unlimited Subject Category 34 Distribution: Nonstandard Availability: NASA-CASI (301) 621-0390			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) Validity of the assumptions relating the applicability of continuum shell theories to the global mechanical behavior of carbon nanotubes is examined. The present study focuses on providing a basis that can be used to qualitatively assess the appropriateness of continuum-shell models for nanotubes. To address the effect of nanotube structure on their deformation, all nanotube geometries are divided into four major classes that require distinct models. Criteria for the applicability of continuum models are presented. The key parameters that control the buckling strains and deformation modes of these classes of nanotubes are determined. In an analogy with continuum mechanics, mechanical laws of geometric similitude are presented. A parametric map is constructed for a variety of nanotube geometries as a guide for the applicability of different models. The continuum assumptions made in representing a nanotube as a homogeneous thin shell are analyzed to identify possible limitations of applying shell theories and using their bifurcation-buckling equations at the nano-scale.				
14. SUBJECT TERMS carbon nanotubes, mechanical behavior, elasticity, buckling modes, scaling laws			15. NUMBER OF PAGES 21	
			16. PRICE CODE A03	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT	